

Wigner function's exact and numerically effective propagator

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Exploiting alternative representations for the Wigner function's dynamical equation, we develop a general strategy for effective numerical propagation. As an example, the split-operator approach is implemented and illustrated for a variety of systems.

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The Wigner function was introduced at the dawn of quantum mechanics [1] resulting in a powerful tool to analyze the quantum-classical transition [2–4]. The Wigner function's dynamic equation, known as the Moyal's equation of motion [5, 6], can be written as either a partial differential equation containing infinite-order derivatives, or an integro-differential equation. Hence, development of efficient numerical methods has been hindered by the equation's inherent complexity.

Many different numerical methods were proposed based on solving the integral representation of the Moyal's equation [7–10], reducing to an effective Boltzman transport equation [11, 12], propagating Gaussian and coherent states [13–15], combining spectral methods with optimization techniques [16], *etc.*

Moyal's equation of motion is [17]

$$\frac{\partial W(x, p)}{\partial t} = \{ \{ H(x, p), W(x, p) \} \}, \quad (1)$$

where $\{ \{ , \} \}$ denotes the Moyal bracket. An explicit expansion of the bracket leads to

$$\begin{aligned} \frac{\partial W(x, p)}{\partial t} &= \frac{2}{\hbar} H(x, p) \sin \left(\frac{\hbar}{2} \overleftarrow{\partial}_x \overrightarrow{\partial}_p - \frac{\hbar}{2} \overleftarrow{\partial}_p \overrightarrow{\partial}_x \right) W(x, p) \\ &= \frac{1}{i\hbar} H(x, p) \left(e^{\frac{i\hbar}{2} \overleftarrow{\partial}_x \overrightarrow{\partial}_p - \frac{i\hbar}{2} \overleftarrow{\partial}_p \overrightarrow{\partial}_x} - e^{-\frac{i\hbar}{2} \overleftarrow{\partial}_x \overrightarrow{\partial}_p + \frac{i\hbar}{2} \overleftarrow{\partial}_p \overrightarrow{\partial}_x} \right) W(x, p) \\ &= \frac{1}{i\hbar} \left[H \left(x + \frac{i\hbar \partial_p}{2}, p - \frac{i\hbar \partial_x}{2} \right) - H \left(x - \frac{i\hbar \partial_p}{2}, p + \frac{i\hbar \partial_x}{2} \right) \right] W(x, p), \end{aligned} \quad (2)$$

which can be expressed in terms of the generator of motion \hat{G} as

$$i\hbar \frac{\partial W(x, p)}{\partial t} = \hat{G} W(x, p), \quad (3)$$

$$\hat{G} = H \left(\hat{x} - \frac{\hbar}{2} \hat{\theta}, \hat{p} + \frac{\hbar}{2} \hat{\lambda} \right) - H \left(\hat{x} + \frac{\hbar}{2} \hat{\theta}, \hat{p} - \frac{\hbar}{2} \hat{\lambda} \right), \quad (4)$$

where the operators $\hat{x}, \hat{p}, \hat{\theta}, \hat{\lambda}$ satisfy the following commutator relations [18]

$$[\hat{x}, \hat{p}] = 0, \quad [\hat{x}, \hat{\lambda}] = i, \quad [\hat{p}, \hat{\theta}] = i, \quad [\hat{\lambda}, \hat{\theta}] = 0. \quad (5)$$

Note that Eq. (3) contains no direct reference to specific differential operators.

The generator of motion for the Hamiltonian $H = \frac{\hat{p}^2}{2m} + U(\hat{x})$ reads

$$\hat{G} = \frac{\hbar}{m} \hat{p} \hat{\lambda} + U(\hat{x} - \hbar \hat{\theta}/2) - U(\hat{x} + \hbar \hat{\theta}/2). \quad (6)$$

Moyal's equation (1) is recovered in the phase space representation $x - p$ for which

$$\hat{x} = x, \quad \hat{p} = p, \quad \hat{\lambda} = -i\partial_x, \quad \hat{\theta} = -i\partial_p. \quad (7)$$

Utilizing an alternative representation in the $x - \theta$ space

$$\hat{x} = x, \quad \hat{p} = i\partial_\theta, \quad \hat{\lambda} = -i\partial_x, \quad \hat{\theta} = \theta, \quad (8)$$

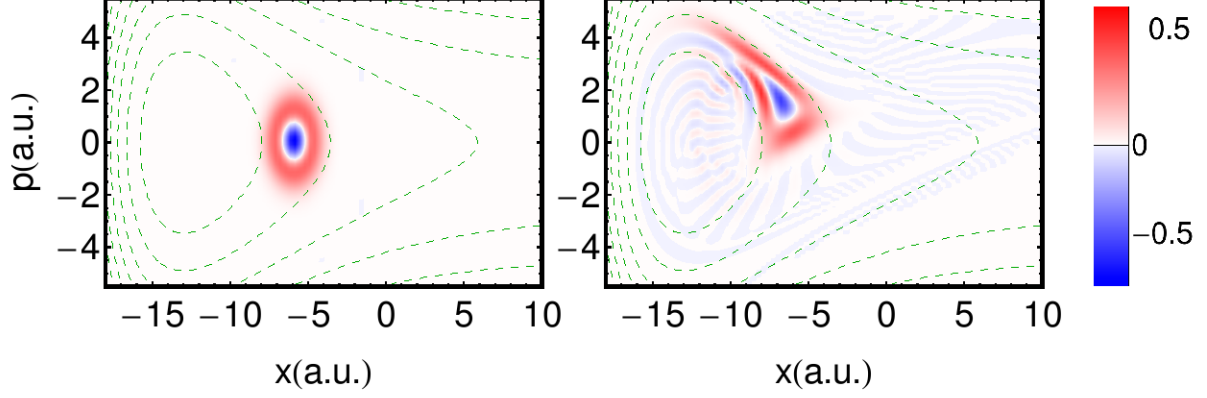


FIG. 1: The evolution of the Wigner function at times $t=0$ a.u. and $t=7.5$ a.u. for the Morse potential $U(x) = 20(1 - e^{-0.16x})$. The initial state corresponds to the first excited state of the Harmonic oscillator.

the equation of motion turns into

$$i\hbar \frac{\partial B(x, \theta)}{\partial t} = \left[\frac{\hbar}{m} \frac{\partial^2}{\partial \theta \partial x} + U\left(x - \frac{\hbar\theta}{2}\right) - U\left(x + \frac{\hbar\theta}{2}\right) \right] B(x, \theta), \quad (9)$$

where the underlying Wigner function is recovered through a Fourier transform

$$W(x, p) = \int d\theta e^{ip\theta} B(x, \theta). \quad (10)$$

Moreover, there are two additional representations in terms of the $\lambda - \theta$ and the $\lambda - p$ variables. The corresponding representations of the quantum state $Z(\lambda, \theta)$ and $A(\lambda, p)$ are obtained as

$$Z(\lambda, \theta) = \int dx e^{-i\lambda x} B(x, \theta), \quad (11)$$

$$A(\lambda, p) = \int dx d\theta e^{i(p\theta - \lambda x)} B(x, \theta). \quad (12)$$

The latter transformation is specially important and is hereafter denoted by \mathcal{F} , such that

$$A(\lambda, p) = \mathcal{F}B(x, \theta). \quad (13)$$

In contrast to Moyal's equation (1) in the phase space, Eq. (9) can be numerically propagated by a broad variety of numerical methods developed for the Schrödinger equation. In particular, the first- and second-order split-operator methods given by

$$U^{(1)}(t + \Delta t, t) = e^{-\frac{i\Delta t}{m} \hat{p} \hat{\lambda}} e^{-\frac{i\Delta t}{\hbar} \left[U\left(t, \hat{x} - \frac{\hbar\theta}{2}\right) - U\left(t, \hat{x} + \frac{\hbar\theta}{2}\right) \right]} \quad (14)$$

$$U^{(2)}(t + \Delta t, t) = e^{-\frac{i\Delta t}{2\hbar} \left[U\left(t, \hat{x} - \frac{\hbar\theta}{2}\right) - U\left(t, \hat{x} + \frac{\hbar\theta}{2}\right) \right]} e^{-\frac{i\Delta t}{m} \hat{p} \hat{\lambda}} e^{-\frac{i\Delta t}{2\hbar} \left[U\left(t, \hat{x} - \frac{\hbar\theta}{2}\right) - U\left(t, \hat{x} + \frac{\hbar\theta}{2}\right) \right]}, \quad (15)$$

can be effectively implemented by utilizing the Fast Fourier Transform from the $x - \theta$ to $\lambda - p$ representation. For example, the first-order propagation takes the form

$$B(t + \Delta t, x, \theta) = \mathcal{F}^\dagger e^{-\frac{i\Delta t}{m} p \lambda} \mathcal{F} e^{-\frac{i\Delta t}{\hbar} \left[U\left(t, \hat{x} - \frac{\hbar\theta}{2}\right) - U\left(t, \hat{x} + \frac{\hbar\theta}{2}\right) \right]} B(t, x, \theta). \quad (16)$$

More details and a Python source code is provided in the Appendix. This method was employed to generate animations of the Wigner function propagation in the case of quartic [19], Morse [20], and Gaussian [21] potentials. In particular, Fig. 1 shows the initial and final state of the Morse potential propagation.

Conclusions. Exploiting the ability to express the time-evolution equation in alternative representations (where the phase space is a special case), we presented an effective and straightforward strategy for the Wigner function propagation. In fact, numerical evaluation is reduced to solving a Schrödinger-like partial differential equation. One of such methods is the spectral split-operator, employed to calculate the evolution for the Morse, quartic, and Gaussian potentials. This method can be generalized to non-unitary evolution. Moreover, a similar numerical approach is applicable to the spinorial relativistic Wigner function [22].

APPENDIX

The following is the Python implementation of the first-order split-operator.

```
#-----Loading packages-----
import numpy as np
import scipy.fftpack as fftpack

#-----Defining the potential-----
def Potential (x):
    return 0.1*x**4

#-----Specifying parameters in atomic units -----

discretizationX = 512      # Number of points in x
discretizationP = 512      # Number of points in p
dt = 0.02                  # time increment
timeStepsN=180             # number of propagation steps
mass = 1.                  # particle's mass
amplitudeX = 9.0           # x range = [-amplitudeX, amplitudeX]
amplitudeP = 25.0          # p range = [-amplitudeP, amplitudeP]
hbar = 1.                  # Planck constant

#-----Defining x_vector, p_vector, theta_vector and lambda_vector-----
#-----containing the respective range of values-----

x_vector = \
    np.linspace(-np.abs(amplitudeX), np.abs(amplitudeX*(1. -2./discretizationX)), discretizationX )

p_vector = \
    np.linspace(-np.abs(amplitudeP), np.abs(amplitudeP*(1. -2./discretizationP)), discretizationP )

theta_vector = fftpack.fftshift( \
    2.*np.pi* fftpack.fftfreq( p_vector.size , p_vector[1]-p_vector[0] ) )

lambda_vector = fftpack.fftshift( \
    2.*np.pi* fftpack.fftfreq( x_vector.size , x_vector[1]-x_vector[0] ) )

#-----Defining X,P,Lambda and Theta grids-----

Theta, X = np.meshgrid (theta_vector, x_vector)
P, Lambda = np.meshgrid (p_vector, lambda_vector)

#-----Defining the propagator factors-----

potentialPropagatorFactor = fftpack.ifftshift( \
    np.exp( -1j*dt*(Potential(X-hbar*Theta/2.) - Potential(X+hbar*Theta/2.)) ), axes=(1,) )

kineticPropagatorFactor = fftpack.ifftshift( \
    np.exp( -1j* Lambda*P*dt/mass ) , axes=(0,))

#-----Secifying the initial state-----

W_init = np.exp( -(X-2)**2 - (P )**2) + 0j

#-----Propagation-----

W = np.array( W_init)

for t in range(1,timeStepsN):
    # Transforming to the X-Theta representation
    B = fftpack.fft(W, overwrite_x=True, axis=1)

    # Applying the factor associated with the potential
    B *= potentialPropagatorFactor

    # Transforming to the Lambda-P representation
    Z = fftpack.fft(B, overwrite_x=True, axis=0)
    A = fftpack.ifft(Z, overwrite_x=True, axis=1)
```

```

# Applying the factor associated with the kinetic energy
A*= kineticPropagatorFactor

# returning to the X-P representation
W = fftpack.iffth(A, overwrite_x=True, axis=0)

W_final = W

#-----Ploting the final state in the Python SAGE distribution (www.sagemath.org)-----
matrix_plot( np.array(W_final.real) , cmap='hsv', colorbar=True, origin='lower')

```

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